New proposal

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Management of a hydrogen-based decentralized energy supply system using multi-agent reinforcement learning

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1. Basic information

1.1. Title

Management of a hydrogen-based decentralized energy supply system using multi-agent reinforcement learning

1.2. Keywords

Decentralized energy supply system; Reinforcement learning; Machine learning; Sustainability

1.3. Abstract

The exploration of energy sources close to the location where they will be used is referred to as decentralized energy supply systems (DESS). It has become an attractive option for industries, for reasons of sustainability, energy cost reduction, and resilience to energy shortages. The conversion of electrical energy into hydrogen is particularly suitable in such cases, as it enables medium to long-term storage. However, the existing approaches to systematically control the energy flows in the DESS do not account for the dynamic changes in a manufacturing system. The collaborative project outlined in this proposal aims to investigate how the management of a hydrogen-based DESS can be accomplished using a multi-agent reinforcement learning (MARL) approach. The use of MARL allows the decomposition of the complex optimization problem into smaller subproblems and is therefore expected to provide good solutions for energy management. For this purpose, it will be investigated how the MARL approach is to be designed. Key contributions are the investigation of how the number of agents influences the overall performance and the explainability of this approach.

1.4. Institutions

This is a new proposal for joint research with international cooperation. It was elaborated within the scope of the DFG – CAPES Collaborative Research Initiative – (PIPC), Call 33/2023. In institutional terms, the universities cooperating in this proposal are Federal University of Rio Grande do Norte, in Brazil, and the University of Kaiserslautern-Landau (RPTU), in Germany. The Federal University of Rio Grande do Norte (UFRN) was founded in 1958, on June 25th. Its main campus is in the city of Natal, in the state of Rio Grande do Norte, and currently has more than 200 courses and over 43,000 students. RPTU was founded at the beginning of 2023, by merging two universities located in the German state of Rhineland-Palatinate, the Technische

Universitaet Kaiserslautern and the Universitaet Koblenz-Landau. It has about 20,000 students and offers around 160 degree programs.

The present proposal represents the version of the Brazilian research group, to be applied for funding from the Coordination for the Improvement of Higher Education Personnel (Fundação Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – CAPES). Accordingly, another version of this project proposal, parallel in terms of content, matter, and efforts, is to be submitted by the German research group to the German Research Foundation (Deutsche Forschungsgemeinschaft – DFG).

1.5. Applicants

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1.6. Introduction

For reasons of sustainability, energy cost reduction, and resilience to energy shortages companies are increasingly deploying decentralized energy supply systems (DESS). This involves the systematic control and improvement of energy use in a manufacturing system intending to reduce energy consumption and the associated environmental impact by continuously improving energy efficiency through the storage and use of energy at the most opportune time [BMU20]. The conversion of electrical energy into hydrogen is particularly suitable, as it enables medium to long-term storage and has advantages over the sole use of battery technologies for this period [Kalc23]. Furthermore, fluctuations in the availability of renewable energies can be better compensated [Lube22]. Technological advances have made electrolyzers, storage systems, and fuel cells commercially viable for use by private companies. However, existing approaches do not account for dynamic changes within boundary conditions because they consider only static and comprehensively described systems [Cao23]. Moreover, they are limited concerning the considerable complexity resulting from multiple subsystems, decision variables, and constraints. Therefore, a novel approach is needed that considers the expected share of renewable energy, energy costs, and energy demand to decide when to draw energy from which source, store it in the form of hydrogen or electrical energy, or convert it back to electrical energy to power the production system.

The collaborative project outlined in this proposal aims to investigate how the management of a hydrogen-based DESS can be realized using a multi-agent reinforcement learning (MARL) approach. The use of MARL allows the decomposition of the complex optimization problem into smaller subproblems and is therefore expected to provide good solutions for energy management. For this purpose, it will be investigated how the MARL approach is to be designed. Key contributions are the investigation of how the number of agents influences the overall performance and the explainability of this approach.

In literature, several different solutions for controlling a DESS are available. On the one hand, there are several approaches focused on providing the necessary inputs to the energy management algorithms used to control the DESS. Mellit et al. use a deep-learning neural network to provide an accurate prediction of the available photovoltaic power [Mell21]. Rodríguez et al. forecast the short-term wind power density and use an artificial neural network for optimizing a microgrid control [Rodr20]. Windler et al. used a deep feedforward neural network to construct a model for forecasting day-ahead electricity prices on the German and Austrian European power exchanges, with a forecast horizon of up to one month [Wind19].

On the other hand, an important branch of research focuses on determining the optimal capacity of individual subsystems, as in [Hass20]. Qiu et al. contribute to optimize subsystem capacities, with a focus on reducing electricity costs and improving supply reliability [Qiu21].

An approach to control a microgrid using an evolutionary algorithm is provided by Teo et al., who developed a fuzzy-based energy management system [Teo21]. In this case, the microgrid only uses short-term storage in the form of a battery, which is why the complexity, number of variables, and constraints are way lower than in the case of a hydrogen-based DESS. The same limitation holds for the multi-objective optimization of a microgrid published by Li et al. [Li19]. Mah et al. present a PSO-based approach for optimizing energy flows within a DESS that includes various components such as solar panels, electrolyzers, hydrogen storage, fuel cells, and batteries. Their methodology includes energy management strategies that prioritize either hydrogen or battery storage replenishment. This means that, depending on which strategy is initially selected, either the battery or the hydrogen storage will be charged first, even if charging the other storage at a particular time would result in a better solution. Therefore, the limitation of this approach lies in its fixed optimization strategies, which lack adaptability to the dynamic circumstances of real-world applications [Mah21]. Sachs and Sawodny give an example of a MIP approach optimizing an island microgrid for rural areas, which is not connected to the public grid. Therefore, it is supported by a diesel generator and stores energy in a battery. As before the solution space is smaller than in the case of a hydrogen-based DESS due to the number of subsystems. Additionally, the paper focuses only on two target dimensions, cost and robustness [Sach16].

2. Objectives, method, and impact markers

The overall objective of this collaborative project is to develop a MARL approach to control a hydrogen-based DESS capable of reducing energy costs, improving sustainability, and offering resilience against energy shortages to manufacturing systems.

2.1. Objectives

The considered energy supply system consists of an electrolyzer, a hydrogen storage tank, a fuel cell, and a battery. Such a system offers manufacturing companies the possibility to manage their energy supply autonomously and within optimized conditions. A hydrogen-based DESS is therefore required to make the best possible decisions for the company in terms of the Key Performance Indicators (KPIs) of cost, sustainability, and ensuring energy availability to avoid production downtime. The MARL approach to be developed is linked to DTs that augment and control the subsystems of the DESS using simulations to obtain the required state information. Since energy supply has a significant impact on several KPIs of companies, the MARL approach will address multi-objective optimization. For the defined DESS, all parameters characterizing the subsystems will be considered as inputs for the MARL approach to ensure transferability to systems with different characteristics of the specific subsystems. The most relevant results of the outlined project are expected with respect to the field of MARL for energy management, the influence of the number of agents on the DESS performance, and the explainability of the application of MARL.

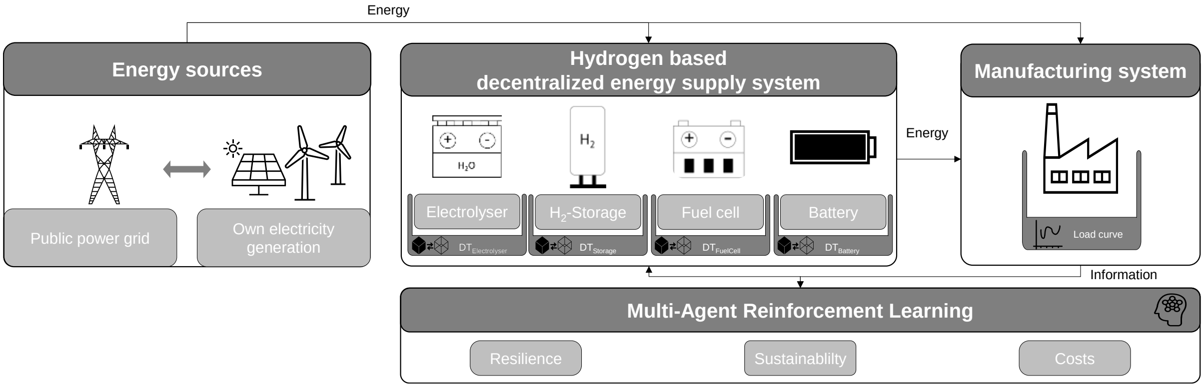

Figure 1: Connection of DESS, DTs and the MARL approach for controlling energy flows

To achieve the overall objective, the three following sub-goals are to be investigated:

1) Utilization of DTs and development of a framework to enable the control of the DESS with a MARL approach;
2) Investigation of the performance of different MARL approaches for the management of the DESS;
3) Assurance of the transferability of the project results.

2.2. Method

A short description of how the three aforementioned subgoals will be attained is given below. A detailed description of the methodology is provided in section 4, together with specific goals.

Subgoal 1: To investigate the potential of MARL for the control of the DESS, an environment must be developed that provides the necessary information and enables the subsystems to be controlled. The use of DTs is suitable for this purpose. Thus, it is necessary to develop a framework that considers the coupling of DTs with the manufacturing and energy supply system and at the same time addresses the integration of the DT with the MARL approach. The required model inputs of the DTs and the resulting outputs are derived from the structure of the MARL approach.

Subgoal 2: To implement efficient control for DESS, the design of the MARL approach that leads to the best performance will be elaborated. Firstly, different MARL approaches are developed and compared. The optimal number of agents, different agent types, and reward functions are analyzed for their effects on DESS performance. The goal is to develop an optimized MARL approach that can be applied to numerous application scenarios with the aforementioned setup and thus provide added value for hydrogen-based DESS. Furthermore, investigating the explainability of the MARL approach also helps to build user confidence and identify potential errors or opportunities to improve MARL-based DESS.

Subgoal 3: The third subgoal is to ensure that the results obtained for energy management are not tied to specific characteristics of the energy supply and manufacturing systems, but also apply independently. To ensure the general applicability of the MARL approach, typical scenarios from Germany and Brazil will be selected to develop and validate the approach. In addition, a digital, interactive guideline will be developed that explains how to adapt the parameters to specific energy supply systems and enables users without extensive programming experience to use the approach for new planning tasks.

2.3. Impact

2.3.1. In the field

From a German point of view, the topic of sustainable, decentralized energy supply is of particular interest, as the European Commission's Energy Efficiency Directive (Directive 2012/27/EU), which came into force in 2012, obliges companies in the European Union (EU) to take measures to promote energy efficiency and achieve energy savings [Euro12].

The production and use of hydrogen as part of an energy supply system is also of interest from a Brazilian perspective, as it allows for avoiding periods of energy shortage, as electricity supply is not guaranteed for about 12.77 hours per year (compared to 10 minutes in Germany) [Verb22, Souz21]. Especially in the north of Brazil, the high solar radiation and constant winds provide an opportunity to convert renewable energy into hydrogen. In addition, the use of a hydrogen-based DESS can reduce carbon emissions by maximizing the amount of renewable energy used in a manufacturing system and allowing excess hydrogen to be sold. Furthermore, due to the higher solar intensity in Brazil, it is assumed that the conditions for own energy production are respectively better (Kaiserslautern, Germany: 1025 kWh/m^2; Natal, Brazil: 1848.5 kWh/m^2) [Worl24].

Finally, this project is expected to expand the applicability of reinforcement learning toward a challenge of structural importance. Such expansion contributes to a better understanding of the potential and limitations of the tools and algorithms used. The gain in visibility also attracts new research to the subject, as well as to the field of machine learning.

2.3.2. In Innovation

As described, most approaches do not consider all three target dimensions (cost, sustainability, and resilience) simultaneously, focus mainly on static conditions rather than dynamic real-world applications, or consider only a subset of the DESS subsystems. The need for a novel approach that has advanced data processing capabilities to accommodate the dynamic characteristics of the energy landscape and to enable autonomous, adaptive, and optimized DESS control is evident. The main purpose of the present proposal is to contribute as a pioneer and with joint efforts to unleash the full potential of DESS, by developing an innovative management concept with unprecedent flexibility in terms of digitalization, autonomy, and optimization.

2.3.3. In the international cooperation

In addition to consolidate the respective core competencies of the German and Brazilian research groups, this project represents an excellent opportunity to cooperate and exchange knowledge in the areas of manufacturing technology, especially in the field of digital twins and reinforcement learning, so that both research groups can improve their competencies.

In the Brazilian side, at the Federal University of Rio Grande do Norte, the Laboratory of Materials Processing by Plasma, under the supervision of the Brazilian coordinator applicant, is currently being expanded to perform investigations on the production of green hydrogen via plasma. As a result, this project will also work as an umbrella for additional lateral projects related to this theme, and attract students interested in international experiences from both undergraduate and graduate levels. During the project, an intensive intercommunication of the results between the research groups will be ensured. Therefore, extensive use will be made of modern communication equipment and weekly online meetings. In this way, expertise will be shared, and experiments will be carried out together in the respective institutes to consolidate the research activities. The exchange of research results from the very beginning of the project will lead to results that cannot be achieved in individually funded research projects. In addition to this scientific benefit, the already existing exchange of students, masters, and engineers from Germany and Brazil will be intensified.

To support and train the Brazilian doctoral students, in particular, during their stay in Germany, RPTU offers various support programs to promote internationalization and to support international students:

- ✓ The Association for International Understanding, Culture, and Education at RPTU e.V. (VKB e.V.) offers language courses for foreign students to help them improve their English and German language skills and better integrate into the academic community.

- ✓ Weekly meetings are organized to promote international cooperation and exchange of expertise between students from different countries and disciplines.
- ✓ "TU-*Nachwuchsring"*, a central organization for the support of young researchers, offers events focusing on career planning and professional development, covering topics such as scientific writing, presentation techniques, and networking across faculties. By participating in these events, Brazilian students can gain valuable insights into the German academic landscape, develop their professional skills, and build connections with peers and mentors.

These comprehensive support measures attest the commitment of the RPTU Kaiserslautern to fostering a welcoming and inclusive environment for international students, enabling them to thrive academically and professionally while pursuing their studies in Germany.

Furthermore, the doctoral students involved in the project will be supported in their personal development. To this end, both the German and Brazilian doctoral students will receive valuable advice on their projects, publications, and doctoral thesis from the professors of the other research group. In addition, the doctoral students will participate in weekly meetings to learn how to work in an international environment and coordinate collaborative projects. Guest lectures by the professors are planned in both countries during the work missions so that the students can also benefit from this international cooperation.

Besides, it is important to mention that two more professors, Prof. Thércio and Prof. Ana Cysne, will be visiting the German partners in person for the very first time. Considering that successful international cooperations are essentially based on a person-to-person level, this represents a substantial enlargement of the contact between the two research institutes.

3. Justification of the partnership UFRN & RPTU

The applying project consortium, comprised of the Institute for Manufacturing Technology and Production Systems (FBK) and researchers of the Federal University of Rio Grande do Norte (UFRN), has previously collaborated extensively in the two projects: "Manufacturing System Models for Industry 4.0 based on highly heterogeneous and unstructured data sets" and its consecutive project "Investigating the applicability of hybrid digital models for manufacturing systems under varying model input conditions." The focus of those collaborations has been on researching topics related to the application of DT in Industry 4.0 environments and hybrid models [Wagn24a, Lang22b]. Among other aspects, these projects have explored the optimization of energy management to supply a model-scale factory either directly from the grid or via a battery using RL. This optimization considers real-time pricing intending to minimize energy costs [Yi22]. Furthermore, sustainability aspects were explored through the utilization of hybrid models in the course of this collaboration [Wagn24b]. In particular, the projects mentioned above focused on hybrid models, which are a combination of physics-based and data-driven models. This enabled both groups to extend their expertise in both types of modeling. Noteworthy is, for example, the combined consideration of kinematic simulations in conjunction with artificial neural networks [Sous20].

In parallel to the works carried out in cooperation and co-authorship with the German applicant, involving DTs, HMs, and ANN and Industry 4.0, the research team of the Brazilian applicant has expertise in machine learning [Jess18, Araú15, Mene18], robotics [Fern20, Ribe18], data analyses [Marq22, Simo20], and in materials science, including hydrogen production [Mede21, Mede19, Mede16]. Noteworthy is that coordinator of the Brazilian applicant has a proposal of post-doc supervision currently under evaluation by the Brazilian National Research Council (CNPq), Call N°32/2023, focused on the production of Green Hydrogen by using Dielectric-barrier discharge (DBD) plasma [Naeet24], [Souz23].

Besides this, the FBK has extensive knowledge in the field of DT [Glat21], as well as in sustainability research in manufacturing [Auri18], and the development of energy management systems [Schw23, Ilse17]. In addition to these projects, the German group, coordinated by Prof. Jan C. Aurich, relies on prior knowledge in the field of analysis and modeling of elements in manufacturing systems and their interactions. In the International Research Training Group IRTG2057 "Physical Modelling for Virtual Manufacturing Systems and Processes" (FKZ: GRK 2057/1), sub-models of the manufacturing system at process, machine, and factory level were researched with a focus on physical properties, conventional, and sustainability-related objectives. The IRTG was driven by the departments of mechanical engineering and computer science and addresses a direct link between digital data models and engineering planning approaches. Among other things, automated factory layout planning was investigated using RL, resulting in comprehensive competencies concerning the modeling of layout planning and the evaluation of layout variants using discrete event material flow simulations in combination with RL [Klar23b]. As part of this project, the applicant was able to expand its extensive expertise in the application of RL to production-related use cases at the factory level. The results of a broader study imply that the best-performing RL agent can generate layouts that are comparable to or better than the best solution generated by a meta-heuristic [Klar23a]. This included the evaluation of more than 10 fully implemented RL approaches and their comparison with the results of metaheuristics. Consequently, RL is the subject of numerous and diverse research studies by the German applicant, including cases focused on other than layout planning, such as on value stream design [Lang22a], and regarding the explainability of RL [Klar24].

4. Methodology

4.1. Funding period I

All tasks to be carried out in this project were organized into six main work packages (WPs) for the first funding period and four work packages for the second period. As the German cooperation partner has to submit another proposal for the second funding period, only the first funding period is described in detail here. For the second funding period, both groups will evaluate the results from the first funding period together and adjust and detail the work plan for the second funding period. The work packages for funding period one are listed and described in detail below.

WP 1: Modelling of the object of investigation

Specific goal: Definition of investigation objects, development of an evaluation model, framework incorporating energy supply system with digital twins and MARL for DESS

WP 1.1: Definition of the investigation objects and modeling of energy availability

The first sub-task involves defining three different scenarios (see Table 3). These scenarios cover the different characteristics of energy supply in Germany and Brazil, different optimization goals, and compositions of the DESS. Major differences between these two countries are the reliability of the public energy grid, the primary energy used, and the availability of renewable energy for private energy production. The Brazilian average amount of renewable energy within the power grid is about 86 %, while the average amount in Germany is about 52 % [Sphe23]. This means that the environmental impact of using energy from the public power grid varies. Another difference is the reliability of the public power grid: With a downtime of about ten minutes per year, the power grid in Germany is one of the most reliable in the world, while Brazil has a downtime of 12.77 hours per year [Verb22, Souz21].

Three productions scenarios were selected to represent the demands of a large number of companies (single-piece, small, and large series production). This is necessary as e.g. the energy demand of a single-piece production is more volatile than in a large series production. In contrast, large series production usually requires much more energy. The size of the company therefore has an impact on the total consumption and the load curve. For each scenario, three energy load curves are synthesized for a single-piece, small, and large series production based on VDI 4655. Since the physical processes of the DESS subsystems are known and their behavior can be sufficiently simulated, the use of synthetic data is valid. The transferability to real systems can thus be ensured.

Two of the three scenarios represent the Brazilian characteristics. Due to different public energy grid reliabilities one scenario covers companies in a sparse (public grid has a high risk of failure) and one in a densely populated area (public grid has a low risk of failure) with the corresponding infrastructure and therefore target for using the DESS. The third scenario focuses on companies located in Germany. Due to its homogeneity of the energy supply (compared to Brazil), only one scenario for Germany is defined. To analyze the different scenarios, different target weighting in terms of resilience, sustainability, and costs will be investigated according to the differences between these locations and their need for resilient, cost-efficient, and sustainable production. Considering these scenarios ensures that the MARL approach applies to a large number of different industries with different requirements.

Table 1 – Main scenarios under investigation

	Scenario 1	**Scenario 2**	**Scenario 3**
Location	Brazil (low grid reliability)	Brazil (high grid reliability)	Germany
Main target	Resilient production	Sustainable and cost-efficient	Sustainable and cost-efficient
Amount of renew-able energy (grid)	High	High	Low
Reliability of the power grid	Low	High	High
Production type	Single-piece, small and large series	Single-piece, small and large series	Single-piece, small and large series

Furthermore, energy availability and cost forecasts are considered, which take into account both fossil and renewable energy sources from the public grid as well as renewable energy sources from own energy generation, such as photovoltaics. Historical energy availability data that are derived from Geographical Information Systems (GIS) and energy cost data derived from the SMARD (Electricity Market Data for Germany) and ANEEL (Brazilian National Agency for Electric Energy) database on a representative time frame serve as surrogates for forecast models.

WP 1.2: Formulation of an evaluation model

The focus of WP 1.2 is to develop an evaluation model for assessing the performance of the DESS, taking into account the conflicting priorities between resilience, costs, and sustainability. The evaluation model has to consider factors such as grid reliability, renewable energy availability, and energy cost. In addition, different shares of renewable energy from own and public supplies are included in the analysis. The model also considers the differences between Germany and Brazil caused by different grid reliability and its share of renewable energies.

Based on a scenario analysis the evaluation model integrates the scenarios defined in WP 1.1 and thus provides a tool for comparing and evaluating the strategies for achieving the associated targets. The target dimensions are parameterized and mathematically formalized for the development of the evaluation model that serves as a basis for the reward function of the agents of the MARL, which in turn serves as a basis for WP 3 and 4.

WP 1.3: Development of a MARL framework

The third subtask focuses on the development of a MARL framework. To effectively use MARL for the management of DESS, it is crucial to ensure a seamless integration between the DESS subsystems, their DTs, and the individual agents. The DESS subsystems include the electrolyzer, hydrogen storage, fuel cell, and battery, as well as energy sources such as solar, wind, and grid. These are connected to digital twins that provide the digital inputs and outputs (I/Os) of the physical system to the agents, which will be integrated into different MARL approaches. Hence, a detailed analysis of the MARL system requirements, including data sources, communication protocols, and decision-making processes is performed. Based on Systems Modelling Language (SysML), the flow of information and data is modeled in Unified Modeling Language (UML) for different compositions of MARL approaches (e.g. various numbers of agents).

WP 2: Development and implementation of DTs and the RL environment

Specific goal: Development and implementation of DTs and connection to the MARL approach.

WP 2.1: Development of DTs for accurate DESS representation

In the first step, DTs will be developed and implemented to replicate the behavior of real-world components (electrolyzer, storage, fuel cell, and battery) within the DESS. The information within the DTs forms the base for the MARL approach. As the inputs to the MARL, which are derived from the DTs are different for each scenario, they need to be defined accordingly. Table 2 shows the I/Os and the action space used for this purpose. The electric battery can store, charge, or discharge its energy. The I/Os represent the charge and discharge curves. The electrochemical conversion in the electrolyzer and fuel cell can be controlled between zero and full load, with hydrogen and electrical energy representing the I/O variables. The hydrogen tank is closely coupled to the fuel cell and electrolyzer. Building on the laws of thermodynamics this results in a charge and discharge curve. The aggregated factory load curve is considered as an additional input to the MARL approach (a detailed consideration will follow in the second funding period). Models and simulations of the behavior of the DESS-subsystems will be implemented and serve as a central tool for testing and validating the MARL approach, providing a controlled environment for assessing the performance and robustness of the interconnected systems. The implementations of the DTs serve as the basis for the MARL environment, simulating the behavior of real systems. This ensures transferability to real applications in which the DTs serve as an interface to the subsystems of the DESS.

Table 2 – Actions and I/O's of the digital twins

Digital twin	Actions	In- and Outputs
Battery	Charge, discharge, hold	Discharge curve
Fuel cell/electrolyser	On/off; 0-100%	$H_2 \leftrightarrow$ Electrical power
H_2-storage	Charge, discharge, hold	Discharge curve
Factory		Load profile

WP 2.2: Development of data exchange interfaces

To provide the relevant inputs to the MARL approach, communication channels between DTs and the subsystems of the DESS and MARL will be developed to ensure a seamless exchange of information. The aim is to ensure a cohesive network that enhances the collaborative nature of the DT and MARL framework.

For this purpose, the DESS subsystems and interfaces, as described in the framework (WP 1.3), will be integrated into a programming platform. Matlab® is well suited for this purpose, as special models for simulating e. g. fuel cells have already been integrated into Simulink [Abdi16]. This allows both synthetic and real data to be accessed and processed, enabling the MARL approach to make informed decisions based on a comprehensive set of information. As not only data-driven but also physics-based digital twins provide I/Os to the MARL approach, a scalable platform can be achieved that has the corresponding integration capabilities for real data.

WP 2.3: Implementation of the RL environment and reward functions

This work package includes the integration of the digital twins into the RL environment, the development and implementation of reward functions, and the setup of interfaces for the connection to the agents (WP 3). Interfaces to the DTs will be implemented to process the state of the DESS as a result of actions and the value of the reward function. An environment class is implemented that allows the instantiation of scenario-specific environments based on the DTs. This allows to model and study different energy supply configurations of the manufacturing system. Different reward functions (e.g. competitive, cooperative, temporal difference) will be developed to investigate the performance of the MARL approach based on different reward functions in WP4. The reward functions will be developed based on the evaluation model (WP 1.2). This allows the weighting of objectives in terms of prioritization (sustainability, resilience, cost). In addition, the energy purchased from the public grid to cover gaps in the energy supply is considered in the reward function. The results of this WP are implemented reward functions and configurable environments. The environments are adapted to the respective energy supply configuration and the energy demand behavior of the objects of the scenarios.

WP 3: Development and improvement of RL agents for the management of a DESS

Specific goal: Utilization of DTs and RL as part of a DESS

WP 3.1: Conception and implementation of different RL agents for the DTs

Since each decision process of the respective agents of the MARL approach differs in its action space as well as in its data structure, preliminary experiments will be performed in WP 3.2 for each subsystem of the DESS (electrolyzer, hydrogen tank, fuel cell, and battery). To compare different learning approaches of the RL agents, one algorithm from each of the three classes of policy-based, value-based, and hybrid learning algorithms (e.g., Deep Q Learning, Vanilla Policy Gradient, and Actor Critic) will be selected and implemented for each subsystem using the Python library Tensorflow. The parameters of the agents' actions are related to the use of the components of the DESS (e.g., charging the battery storage or extracting energy from the battery storage, see Table 2). As a result of this WP, all agents for the DESS subsystems will be implemented.

WP 3.2: Application and improvement of the agents

The starting point for WP 3.2 is the definition of a design of experiments (DoE) in which the investigation of the multitude of parameters is determined in a structured manner. To reduce the complexity of the problem setting for each agent, the parameters of the other subsystems are not varied during the training. The influence of the hyperparameters of the RL agents (e.g. number of layers, number of neurons per layer, activation functions, agent-specific parameters) on the performance of the approach is compared using the final reward value, the realized loss value, and the convergence behavior. For this purpose, a separate agent is initialized for each hyperparameter combination and trained on the high-performance computing cluster. The result is a defined set of properties for every agent that includes the learning approach and a set of hyperparameters for every agent. The investigations within WP 3.2 are carried out by both groups (Brazil and Germany) initializing the selected representative scenarios from WP 1.1 to ensure a manageable conduction of the experiments. Results from both groups (Brazil and Germany) are tested interchangeably to provide a scalable and generalizable approach.

WP 4: Integration to a MARL approach and performance investigation

Specific goal: Integrated MARL agents to reach the best performing MARL approach for DESS-management

WP 4.1 Training and performance evaluation of the MARL approaches

Since the integration and interaction of the agents within the MARL approach can lead to conflicts between the agents, further investigations on the combined consideration are necessary. Within this WP, the performance of the MARL approach is examined as a dependence on selected configurations, such as the design of the reward function. For this purpose, the designed reward functions (WP 2.3) are evaluated. In particular, global rewards are compared with decomposed rewards. Global reward refers to a single, global reward that is assigned to all agents based on the overall performance of the group whereas decomposed rewards assign individual rewards to each agent based on its own actions or contributions to the collective goal. Both types of reward functions allow different target weightings from the evaluation model (WP 1.2) and can be considered depending on user preference. To reflect these user preferences both research groups will develop MARL approaches covering their scenarios (WP 1.1). In addition, further variable parameters will be selected for each approach, which can be composed as follows: temporal sequence of agent decision making (simultaneous vs. sequential), temporal sequence of agent training (parallel vs. sequential). The identified reward function and the set parameters are fixed and serve as a starting point for further investigations.

WP 4.2: Investigation of the influence of the number of agents on the performance of MARL-based energy management for DESS

Subsequently, the number of agents with the best performance for the problem is determined by successively combining the agents until a single agent is selected for the entire DESS. The successive grouping is achieved by extending the scope of action of an agent through the actions of an agent of another component of the DESS (e.g. an agent performs actions for both the electrolyzer and the fuel cell). For each grouping, the necessary adjustments of the input representations, the state information, and the necessary interaction mechanisms of the agents are implemented. To reduce the complexity and possible combinations, the DoE for the hyperparameters of the grouped agents is reduced based on the results of WP 3. The result is the identified influence of the number of agents within the MARL system for this problem setting and the corresponding identified parameters.

WP 5: Development of explainability methods for the MARL approach

Specific goal: Identified influencing factors of the decision-making process of the MARL approach

The best-performing MARL approach from WP4 serves as the starting point for investigating its explainability. First, the traceability of the sequential decisions of the agents is ensured. Second, appropriate techniques will be implemented to visualize the decision steps and the state changes depending on the states of all components of the DESS. Selected methods (e.g., reward decomposition, occlusion sensitivity, and policy summarization) are developed and applied to identify the factors influencing agent behavior. Borderline cases for the states of the components of the DESS are then defined and the behavior of the MARL is systematically investigated by successively approaching them. Visualization techniques include the presentation of multiple dimensions, such as the varied state of a component, the state of the other DESS components, its behavior over time, as well as other identified influencing factors. In addition, sensitivity analyses are performed on the objective weights within the reward functions to develop an understanding of the behavior of the management system with varying user preferences. Due to the variance in user preferences, cultural influences on the results of the approach can also be evaluated. By analyzing the visualizations, insights into the control behavior of the MARL system can be captured and explained.

WP 6: Evaluation of the transferability of the results

Specific goal: Validation and verification of the previously developed MARL approach for the management of a DESS

The overall results of the previous WPs are summarized in the form of an action guideline, which covers the development of MARL for the energy management of DESS. In addition, the implemented program is prepared in the form of an interactive, digital guideline. To ensure the transferability of the results, the approach is applied to three newly defined application scenarios. These are defined analogously to the approach in WP 1.1 and consider characteristics from both countries. The MARL-based DESS is applied to these scenarios according to the guidelines. For comparison, a conventional rule-based energy management system is implemented to compare the performance of the MARL approach. This is defined by if-else conditions (e.g. when the hydrogen storage level is above 80%, the electrolyzer is operated at full load until the level is below 40%). In this way, the developed approach is benchmarked against a widely used state-of-the-art energy management mechanism. Possible weaknesses of the MARL approach can thus be identified and, if necessary, eliminated in an improvement iteration. The results of the project will be continuously documented. The experiences and results of the research topics as presented in the work program will be summarized in a closing report. Results that are relevant to science and industry will be published in national and international papers that are co-authored by researchers of both groups.

4.2. Funding Period II

Most of the results of funding period I (WP 1-5) serve as input for further research in funding period II, which is composed by the work packages presented below. As explained above, the content of the work packages will be detailed by both groups together after evaluating the results from funding period I.

<u>WP 7: Extension of the object of investigation</u>

• Extension of the object of investigation from the energy supply to the manufacturing system

• Modeling of production system with Five-machine six step mini fab

• Extending the scenarios by adding job information (due date, number of parts, etc) as a basis for energy-based job shop scheduling

• Additional scenario: Energy exchange between companies/production sites in the form of hydrogen or electrical energy

<u>WP 8: Extension of MARL approach: Job Shop Scheduling</u>

• Adding DTs for machines in the manufacturing system providing energy demands

• Extension of the framework from WP 1.3 by adding energy-based job shop scheduling as another task for the MARL approach

• MARL approach manages the energy demand as well as the supply at the same time to provide even better solutions regarding cost, emission, and resilience

• Investigating the performance of the extended MARL approach

<u>WP 9: Explainability of extended MARL approach</u>

• Investigation of transparency, causality, bias, fairness, and safety

• Development of explainable models taking into account core elements of explainable artificial intelligence model performance, interpretable models, and model induction

<u>WP 10: Validation and transferability</u>

• Validation of MARL approach for energy supply management and energy-based job shop scheduling on defined scenarios from WP 6

• Aggregation of results from both funding periods and extension of the interactive guideline

5. Expected Results

The following results for both research groups are expected from the tasks and working packages proposed in this project:

I. The consolidation and improvement of their core competencies by the exchange of knowledge;
II. The nucleation of parallel projects related to this theme, and an increase in the number of students interested in international experiences from both undergraduate and graduate levels;
III. Intensification of academic productions (such as scientific publications, master dissertations and doctoral theses), especially in those with international co-authorship;
IV. Training of human resources from the Brazilian side, by attending the support programs offered by the RPTU to foreign students, especially regarding culture, language skills, international posture, and integration;
V. A substantial enlargement of the contact between the two research institutes;
VI. Scientific insights on the applicability of MARL to manage DESS and Job Shop Scheduling at once.

6. Academic productions

The importance of the subject and the pioneer nature of the approach pose a great potential for sound publications. Due to the innovative content, the topics considered to be the focus of the first publications are: the implementation of the digital twin of the DESS, the connection between DT and MARL, the determination of the most relevant factors affecting the control of the DESS, and the comparative performance of the reinforcement learning algorithm as managing tool for DESS. Altogether, at least the results presented in Table 3 are expected. All of the papers are planned to be elaborated by both research groups together, as a result of collaborative efforts.

Table 3 - Academic productions expected

Type	Quantity (funding periods I and II)
Publications in peer-reviewed journals	4
Publications in peer-reviewed conferences	6
Publication of doctor thesis in the Brazilian side	4
Others (congresses, book chapters, etc.)	4

7. Description of the knowledge incorporation

This project can only be carried out in international collaboration with researchers from the University of Rio Grande do Norte (UFRN in Natal, Brazil). The work distribution (see work program in section 2.3) is as follows: Both research groups work together on the first two WPs, as these form the basis for the subsequent WPs and are generally valid for all subsequently developed MARL variants. WPs 3, 4, and 5 investigate a large number of different variants that could not be investigated by one group alone (different reward functions, agents, agent compositions, number of agents, approaches to explainability). Therefore, the two research groups will work independently in some areas (e.g. the development of a specific agent) in order to cope with the workload. The scientific exchange between the two groups will be ensured by the collaborative activities described in this proposal. This is particularly important to determine which of the approaches promises the best performance for the DESS. This approach will also ensure that there is a broad exchange of knowledge and acquisition of expertise in both groups. The final WP 6 will again be fully collaborative as all results will be combined and validated. The German group is responsible for the development of the MARL approach for the German scenario and the Brazilian group for the Brazilian scenarios. The continuous exchange will ensure that during the course of the project, a single solution will be developed, including the most promising approaches, using the results of both research groups. Furthermore, the interdisciplinary expertise of the German-Brazilian research group will be jointly used to ensure a high generalizability of the developed interactive guideline in WP 6. Since the Brazilian research group of the UFRN has the necessary competencies in the field of hydrogen and the research group of the FBK in the development of RL approaches, the research tasks will be handled in a complementary way.

Once the project has been completed, the research data and program codes developed in the project will be made permanently available for subsequent use in the university's research data repositories on a git repository and published in the form of quality-assured publications.

8. Available infrastructure

Besides the infrastructure of the PPGCEM, for the accomplishment of the research activities, the Brazilian research team counts with the following scientific equipment:

- ✓ Spectrophotometer (Thermo Scientific, Genesis 10UV)
- ✓ Laboratory for metallographic preparations (Precision cutting machine, grinding and polishing heads, optical microscopes and microhardness equipment)
- ✓ Fume hood and centrifuge separator (Quimis)
- ✓ Muffle furnace (Quimis)
- ✓ Gas cylinders (argon, acetylen, oxygen, hydrogen, nitrogen, methane)
- ✓ Customized reactor for oxidative eletroctrolize

- ✓ Four plasma reactors for thin films, including a magnetron sputtering

The German research partners, on the other hand, counts on data analysis systems, simulation softwares, interactive visualization technologies, together with the following items:

- ✓ Access to RPTU Kaiserslautern-Landau high-performance computing center
- ✓ Access to RPTU Kaiserslautern-Landau libraries and laboratories of FBK
- ✓ Deep learning server
- ✓ Access to the 5G Campus Network of RPTU Kaiserslautern-Landau
- ✓ Various CAD and factory planning software
- ✓ Hard- and software for data analysis and simulations
- ✓ CAVE automatic virtual environment
- ✓ Microsoft HoloLens 1 and HoloLens 2 (Mixed Reality Glasses)
- ✓ Learning factory with Industry 4.0 technologies (sensors, actuators, CPPS)
- ✓ Access to research manufacturing system including additive manufacturing machines (laser powder bed fusion and high-speed laser directed energy deposition) and various machine tools (drilling, milling, grinding, turning)

9. Financial compensation from Brazilian and German Institutions

Not applied

10. Research Groups

The full list of researchers from the Brazilian group is presented in Table 4.

Table 4 – Applicants from the Brazilian research group

Name with academic title	Field of research
Prof. Dr. Thércio Henrique de Carvalho Costa	Film deposition, DBD plasma, thermal spraying plasma
Prof. Dr. Ana Paula Cysne Barbosa	Processing and characterization of composites
Prof. Dr. Fábio José Pinheiro Sousa	Digital twins, Data-driven models, Kinematic simulations
Prof. Dr. Orivaldo Vieira de Santana Jr.	Robotics, Machine learning, Artificial intelligence
Prof. Dr. Rodolfo Luiz Bezerra de Araujo Medeiros	Synthesis and Microstructural characterization of materials for the production of green Hydrogen

From the German side, the research group is represented by Prof. Dr.-Eng. Jan C. Aurich, whose research fields are manufacturing technology, production systems, and smart manufacturing.

11. Joint Actions

Intense collaboration and academic exchange between Brazilian and German research partners are planned. As both research groups have experience in collaborating from the two previous projects, the weekly meetings will continue to have a regular exchange of knowledge.

In terms of human development, the main joint initiatives devised to foster the integration between both research groups are summarized in Table 5.

Table 5 – Joint actions for human development

Joint actions for human development	FP I - year 1				FP I - year 2				FP II – year 1				FP II – year II			
	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV
Weekly online meetings																
Feedback on Dissertation thesis for Brazilian doctoral students by German Professor																
Access to courses and support programs from Association for International																
Guest lectures during work missions in Brazil																
Guest lectures during work missions in Germany																

Despite the positive experiences and the progress that could be achieved through online meetings, for the applied funding period, the project partners intend to perform frequent personal on-site meetings to ensure the project's success. Per funding period, two doctoral students from the UFRN will visit the FBK for one year each. The aim is for at least one of the four doctoral students coming to Germany over the two funding periods to be female. In addition, two visits to Brazil will be performed by the German doctoral candidate. Furthermore, per funding period three work missions will be carried out from the UFRN and two from the FBK. Moreover, at least one work mission will be carried out by Prof. Dr. Ana Cysne, a female research partner of this proposal. The mobility calendar is presented in Table 6. Beyond that, both partners will also attend the annual meeting organized by the funding agencies.

Table 6 – Schedule planned for the work and study missions for the two funding periods

International mobility	FP I - year 1				FP I - year 2				FP II – year 1				FP II – year II			
	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV
Academic exchanges from Brazil to Germany (four doctoral students)				I						III						
						II								I		
Work missions to Germany (7-10 days)																
Academic exchanges from Germany to Brazil (doctoral student)																
Work missions to Brazil (7-10 days)																

11.1. Workplan

The work packages defined in section 4 will be accomplished according to the workplan presented in Tables 7 and 8, for the first and second funding periods, respectively.

Table 7 – Project workplan for the first funding period

Work package		1st year												2nd year											
		1	2	3	4	5	6	7	8	9	10	11	12	1	2	3	4	5	6	7	8	9	10	11	12
1	Modelling of the object of investigation																								
1.1	Definition of the investigation objects and modeling of energy availability																								
1.2	Formulation of an evaluation model																								
1.2	Development of a MARL framework																								
2	Development and implementation of DTs and the RL environment																								
2.1	Development of DTs for accurate DESS representation																								
2.2	Development of data exchange interfaces																								
2.3	Implementation of the RL environment and reward functions																								
3	Development and improvement of RL agents for management of DESS																								
3.1	Conception and implementation of different RL agents for the DTs																								
3.2	Application and improvement of the agents																								
4	Integration to a MARL approach and performance investigation																								
4.1	Training and performance evaluation of the MARL approaches																								
4.2	Investigation of the influence of the number of agents on the performance of MARL based energy management for DESS																								
5	Development of explainability methods for the MARL approach																								
6	Evaluation of the transferability of the results																								

Table 8– Project workplan for the second funding period

Work package		1st year												2nd year											
		1	2	3	4	5	6	7	8	9	10	11	12	1	2	3	4	5	6	7	8	9	10	11	12
7	Extension of the DT and MARL: Job Shop Scheduling																								
8	Extension of MARL-approach: Job Shop Scheduling																								
9	Explainability of MARL-approach																								
10	Validation and transferability																								

12. Selection criteria for granting scholarships

In the Brazilian research group, the CAPES scholarships will be granted to candidates selected by an evaluation committee. This committee will be defined by the Brazilian coordinator, who holds a permanent position at the Graduation Program in Materials Science and Engineering (PPGCEM) of the UFRN. Noteworthy is that the PPGCEM has achieved the maximum grade from CAPES in the two last evaluations. Besides the fulfilment of all mandatory requirements established by the CAPES, both in this specific call and in general guidelines defined by the Brazilian Education Ministry, which are eliminatory, the criteria to be considered in the selection process are the quality of the workplan to be accomplished in the foreign facility and previous academic production. Besides, bearing the gender diversity in mind, at least one of the scholarship holders must be female. An ordinance can be issued by the coordinator of the PPGCEM if necessary.

13. Progress indicators

A list of milestones will be used to verify the accomplishment of the tasks along the project. Such a list can be seen in Table 9, and it is composed by all specific objectives, which in turn were extracted from each work package detailed in section 4.

Table 9 – Progress indicators

Milestone	Checking questions
WP1	Is the investigation object defined?
	Is an evaluation model conceived?
	Is a framework incorporating energy supply with digital twins and MARL developed?
WP2	Is a DT implemented?
	Is it connected to the MARL?
WP3	Does the DESS contain DTs and RL?
	Are the implemented RL agents for the DESS subsystems?
WP4	Are the MARL agent integrated?
	Is this the best performing approach for DESS-management?
WP5	Are the influencing factors of the decision-making process identified?
	Are they ranked in terms of relevance?
WP6	Is the validation test carried out?
	Is the performance of the MARL approach for DESS-management confronted against the literature?
WP7	Is the production system with five-machines six step mini fab modeled?
	Does the model consider energy exchange between companies?
WP8	Are the DT for the manufacturing system created?
	Is the MARL approach for managing energy demand implemented?
WP9	Are the following variables evaluated: transparency, causality, bias, fairness, and safety?
	Do the conceived models take into account core elements of explainable artificial intelligence?
WP10	Is the validity of the MARL approach for energy supply checked?

	Is an interactive guideline considering the results from both funding periods altogether produced?

14. Further Relevant Information

The collaboration between the research groups from the UFRN and the RPTU officially started in 2016, when Prof. Fábio Sousa intermediate an International Cooperation Agreement. The document expired in 2021. In the meanwhile, several students carried out academic exchanges, from both RPTU and UFRN. Besides, both research partners proved their vivid cooperation during the annual meeting in 2022 which was hosted by Prof. Aurich in Kaiserslautern, and the annual meeting in 2023 which was hosted by Prof. Sousa at UFRN in Natal, where Prof. Ana Cysne personally attended with her students.

14.1. Results reached by other previous CAPES projects

In the period from 10/2019 to 01/2025, both universities are cooperating in the scope of the Brazilian-German Collaborative Research Initiative on Smart Connected Manufacturing (PIPC) Program. The project is entitled “Manufacturing System Models for Industry 4.0 based on highly heterogeneous and unstructured data sets", which investigates the applicability of hybrid digital models for manufacturing systems under varying model input conditions. The results from this project, which is still in progress, can be seen in the following literature [Glat21], [Lang22b], [Sous20] [Wagn24a] [Wagn24b] [Yi22], [Dant24].

14.2 Budget

Besides the financial support for academic mobilities and scholarships, fundings for consumables and services are also expected by the Brazilian cooperation partners. Those items are listed below in Table 10, and they will be used to carry out laboratory experiments with graduates and undergraduate students for didactic purposes, enhancing the transfer of knowledge. Digital twins are to be developed and validated as part of these laboratory experiments.

Table 10 – Funding requests for consumables

Item	**Category**	**Unitary cost**	**Amount**	**Cost per item**
Mechanical adaptations (Machining and cutting of mechanical components)	Services	R$ 100/hour	10 hours	R$ 1.000,00
Gaseous compound Methane	Consumables	R$ 1.200/cylinder of 1.2 m^3	2 cylinders	R$ 2.400,00

Gaseous compound Argon	Consumables	R$ 1.300/cylinder of 10 m^3	1 cylinder	R$ 1.300,00
Laboratory Analysis (Measurement of physical adsorption)	Services	R$ 120/sample	20 samples	R$ 2.400,00
Chemical compound Ethanol (Pure analytic, 99.5%)	Consumables	R$ 90/liter	10 liters	R$ 900,00
Laboratory glassware	Consumables	R$ 350/kit with 30 pieces	2 kits	R$ 700,00
			Total	**R$ 8.700,00**

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